The exopolyhedral ligand orientation (ELO) in 3-(nitrato-κO)-3,3-bis(triphenylphosphane-κP)-3-rhoda-1,2-dicarba-closo-dodecaborane(11) dichloromethane 2.2-solvate

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Keywords: metallacarboranes; *trans* influence; exopolyhedral ligand orientation (ELO); dodecaborane(11); crystal structure vertex-to-centroid distance (VCD) method; boron–hydrogen distance (BHD) method.

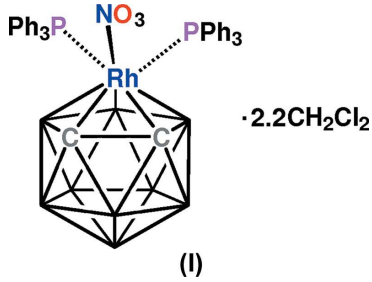
CCDC reference: 1063258

Supporting information: this article has supporting information at journals.iucr.org/c

In the title compound, $[Rh(C_2H_{11}B_9)(NO_3)(C_{18}H_{15}P)_2]\cdot 2.2CH_2Cl_2$, studied as a 2.2-solvate of what was assumed to be dichloromethane, the nitrate ligand lies *cis* with respect to both cage C atoms. Accordingly, the compound displays a pronounced preferred exopolyhedral ligand orientation (ELO) which is traced to both the greater *trans* influence of the cage B over the cage C atoms and the greater *trans* influence of the triphenylphosphane ligands over the nitrate ligand. The overall molecular architecture therefore agrees with that of a number of similar 3-*L*-3,3-*L*′$_2$-3,1,2-*closo*-*M*$C_2B_9H_{11}$ species in the literature.

1. Introduction

Since Hawthorne's first report 50 years ago (Hawthorne *et al.*, 1965), a substantial number of metallacarboranes have been crystallographically characterized, making possible the identification of any patterns in their structures. In this regard, we are particularly interested in the structures of icosahedral 3-*L*-3,3-*L*′$_2$-3,1,2-*closo*-*M*$C_2B_9H_{11}$ species in which the two cage C atoms are adjacent and both bonded to the metal atom, and the exopolyhedral ligand set comprises two different ligands, *L* and *L*′, as part of a conical {*MLL*′$_2$} fragment. Since the *trans* influence of cage C atoms is less than that of cage B atoms, this leads to a distinct conformational preference for the {*MLL*′$_2$} fragment which we have termed exopolyhedral ligand orientation (ELO) (McAnaw *et al.*, 2013). Briefly, if the *trans* influence of *L*′ is greater than that of *L* (*i.e.* the exopolyhedral ligand set comprises two strong ligands plus one weak ligand), the weak ligand tends to lie *cis* to the cage C atoms, whereas if the *trans* influence of *L* is the greater, one of the *L*′ ligands occupies this position.



(I)

The present compound, 3-(nitrato-κ*O*)-3,3-bis(triphenylphosphane-κ*P*)-3-rhoda-1,2-dicarba-*closo*-dodecaborane(11) dichloromethane 2.2-solvate, (I), is an example of a 3,1,2-*M*C_2B_9 metallacarborane with one classically weak ligand (the

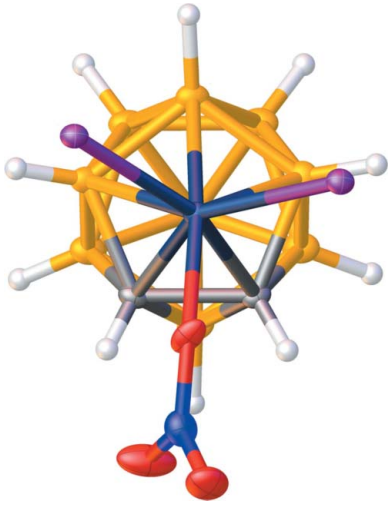


Table 1
Experimental details.

Crystal data	
Chemical formula	$[Rh(C_2H_{11}B_9)(NO_3)(C_{18}H_{15}P)_2]\cdot 2.2CH_2Cl_2$
M_r	1008.69
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	100
a, b, c (Å)	11.2934 (9), 13.0083 (10), 15.8655 (13)
α, β, γ (°)	91.083 (4), 110.514 (4), 99.713 (4)
V (Å^3)	2144.0 (3)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.79
Crystal size (mm)	0.56 × 0.32 × 0.08
Data collection	
Diffractometer	Bruker APEXII CCD diffractometer
Absorption correction	Multi-scan (*SADABS*; Bruker, 2008)
T_{min}, T_{max}	0.660, 0.746
No. of measured, independent and observed $[I > 2\sigma(I)]$ reflections	40881, 10603, 8793
R_{int}	0.035
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.672
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.035, 0.089, 1.05
No. of reflections	10597
No. of parameters	520
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.04, −0.74

Computer programs: *APEX2* (Bruker, 2009), *SAINT* (Bruker, 2009), *SHELXS97* (Sheldrick, 2008), *publCIF* (Westrip, 2010), *SHELXL2014* (Sheldrick, 2015) and *OLEX2* (Dolomanov *et al.*, 2009).

nitrate group) and two stronger ligands (the triphenylphosphane ligands) and so it should belong to the former group. Although the compound was first reported several years ago (Demidowicz *et al.*, 1979), no structural study was carried out. Accordingly, we have resynthesized the compound and, in the present communication, report its crystal structure as the dichloromethane 2.2-solvate with a particular focus of attention being the ELO. Clearly, correct determination of the ELO requires the correct identification of the cage C-atom positions, and to distinguish cage C from cage B atoms we have used the recently reported vertex-to-centroid distance (VCD) method (McAnaw *et al.*, 2013) and boron–hydrogen distance (BHD) method (McAnaw *et al.*, 2014).

2. Experimental

2.1. Synthesis and crystallization

The title compound was prepared by treatment of 3-κ^2-NO_3-3-PPh_3-3,1,2-*closo*-$RhC_2B_9H_{11}$ (Demidowicz *et al.*, 1979) with PPh_3 in diethyl ether, according to the method described in the same paper. Purity was confirmed by elemental microanalysis, mass spectrometry and ^{1}H, ^{11}B and ^{31}P NMR spectroscopies in $CDCl_3$. Orange plate-like single crystals were grown by diffusion of a CH_2Cl_2 solution of the compound and hexane at 243 K.

2.2. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. Initially, all nonmetal cage atoms were described as boron with their attendant H atoms allowed positional refinement. This model (the prostructure) was refined and then analysed by both the VCD (McAnaw *et al.*, 2013) and the BHD (McAnaw *et al.*, 2014) methods. Both methods led to the same conclusion regarding the location of the cage C atoms, specifically that they occupy positions 1 and 2 in the polyhedron. Refinement was completed with cage H atoms continuing to be refined positionally, but with phenyl H atoms set in idealized positions riding on their bound C atom, with C—H = 0.95 Å. For all H atoms, U_{iso}(H) = 1.2U_{eq}(C,B). Attempts to model the disordered CH_2Cl_2/hexane solvent were unsuccessful, so the intensity contribution of the disordered solvent was removed using the *BYPASS* (van der Sluis & Spek, 1990)/*SQUEEZE* (Spek, 2003) procedure, as implemented in *OLEX2* (Dolomanov *et al.*, 2009). The size of the void was calculated to be 388 Å^3, containing approximately 182 electrons. This could correspond to a fractional amount of solvent, *e.g.* 4.4 molecules of CH_2Cl_2 per unit cell. The void is located around a centre of inversion, so there is just one void in the unit cell.

3. Results and discussion

Two molecules per unit cell of 3-κ^1-NO_3-3,3-$(PPh_3)_2$-3,1,2-*closo*-$RhC_2B_9H_{11}$ crystallize in the space group $P\overline{1}$ (Z' = 1), together with disordered solvent that was impossible to model

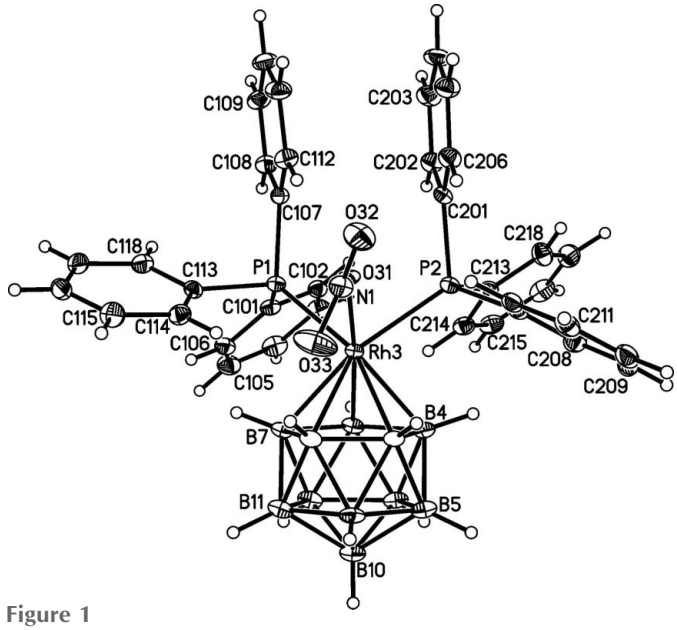


Figure 1
Perspective view of the title compound, showing the atom numbering and with displacement ellipsoids drawn at the 50% probability level except for H atoms. The cage C atoms are shown as boundary ellipsoids, with C1 on the right and C2 on the left.

Table 2
Vertex-to-centroid distances (VCD, Å) and boron–hydrogen distances (BHD, Å) in the prostructure and the final structure of (I).

Vertex	VCD analysis		BHD analysis	
	Prostructure	Final structure	Prostructure	Final structure
1	1.555 (4)	1.571 (3)	0.44 (4)	0.93 (2)
2	1.548 (3)	1.556 (2)	0.22 (4)	0.89 (3)
3	1.717 (3)	1.717 (2)	1.05 (3)	1.07 (3)
4	1.694 (3)	1.695 (3)	1.05 (3)	1.10 (3)
5	1.722 (3)	1.723 (3)	1.08 (3)	1.11 (2)
6	1.701 (3)	1.701 (3)	1.02 (3)	1.02 (2)
7	1.735 (3)	1.736 (3)	1.15 (3)	1.17 (2)
8	1.650 (3)	1.654 (2)	1.10 (3)	1.10 (2)
9	1.683 (3)	1.686 (3)	1.02 (3)	1.02 (3)
10	1.699 (3)	1.700 (3)	1.08 (3)	1.10 (3)
11	1.654 (4)	1.658 (4)	1.12 (4)	1.15 (2)

conventionally, occupying a void of 388 Å^3 per unit cell equivalent to approximately 182 electrons and therefore assumed to be 4.4 molecules of CH_2Cl_2. Nevertheless, the rhodacarborane structure is relatively precisely determined, with the s.u. values on B—B connectivities being typically 0.004 Å. Figs. 1 and 2 show perspective views of the molecule and include the atom-numbering scheme.

Using both the VCD method (McAnaw *et al.*, 2013) and the BHD method (McAnaw *et al.*, 2014), analysis of the prostructure (all cage atoms other than rhodium described as boron and with H atoms allowed positional refinement; Table 2) clearly showed that the cage C atoms are located at vertices 1 and 2, following which these vertices were assigned as C and refinement completed. The correct positioning of the cage C atoms is particularly important in the present case since our main interest in the structure concerns the orientation of the exopolyhedral nitrate ligand relative to the cage C atoms. As is clear from Fig. 2, a view down the Rh3···B10 axis, with phenyl groups omitted for clarity, the nitrate ligand lies *cis* to both cage C atoms, as anticipated, since the *trans* influence of cage C atoms is less than that of cage B atoms and the *trans* influence of nitrate is less than that of triphenylphosphane. The preferred ELO is conveniently quantified by the torsion angle O31—Rh3—cent1—cent2 (θ), where cent1 is the centroid of the C1/C2/B7/B8/B4 carborane face and cent2 is

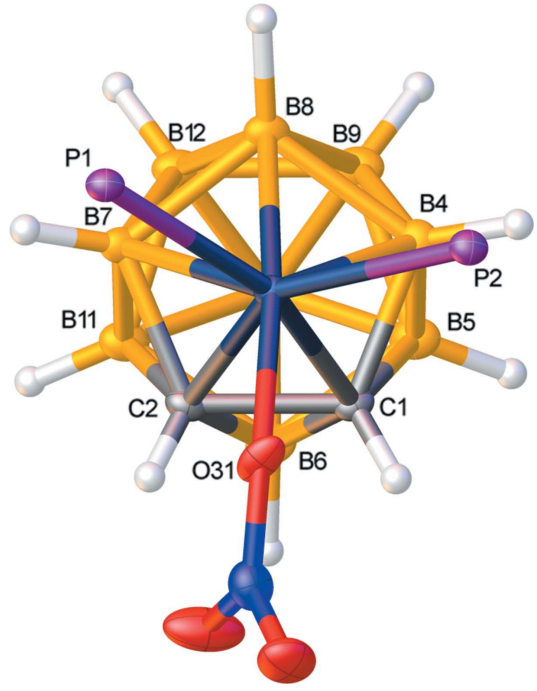


Figure 2
View of the title compound down the Rh3···B10 axis, showing the orientation of the nitrate ligand relative to the cage C atoms. Phenyl groups have been omitted for clarity. Colour code: yellow = B, grey = C, red = O, royal blue = N, dark blue = Rh, purple = P and white = H.

the mid-point of the C1—C2 connectivity. In the title compound, θ is 5.46 (12)°, which is close to the ideal value of 0°.

A search (restricted to structures with no disorder and monodentate exopolyhedral ligands) of the Cambridge Structural Database (CSD; Version 5.35; Groom & Allen, 2014) for icosahedral 3-*L*-3,3-*L*′$_2$-3,1,2-*closo*-*M*$C_2B_9H_{11}$ species in which the metal centre has an 18 valence electron count and the *trans* influence of *L*′ is generally accepted to be greater than that of *L* gives a number of hits. In many, but not all, cases the ligand set is *L*′ = phosphane and *L* = chloride. For these structures, the given positions of the cage C atoms were checked by the VCD method and were correct in all cases. In Table 3, we summarize the hits and list the θ values, calculated

Table 3
Literature 3-*L*-3,3-*L*′$_2$-3,1,2-*closo*-*M*$C_2B_9H_{11}$ species in which ligand *L*′ has a greater *trans* influence than ligand *L*.

The parameter θ (°) is the exopolyhedral ligand orientation (ELO) as described in the text.

CSD refcode	*M*	*L*	*L*′	θ	Reference
CEHCEX	Ru[a]	Cl	PPh_3	−12.9 (3)	Chizhevsky *et al.* (1999)
NITWOC	Rh	Cl	PPh_3	−12.4 (3)	Chizhevsky *et al.* (1997)
TELCIW	Rh	Cl	PPh_3	12.6 (4)	Ferguson, McEneaney & Spalding (1996)
TUBLUX	Co	Cl	PPh_2Me	−15.5 (3)	Hendershot *et al.* (1996)
ZOTVOT	Rh	Cl	PPh_2Me	−9.1 (2)	Ferguson, Pollock *et al.* (1996)
ZOTVIN	Rh[b]	NCMe	PPh_2Me	−8.1 (2)	Ferguson, Pollock *et al.* (1996)
HIZQIQ	Ru	PhC≡CMe[c]	CO	5.5 (2)	Jeffery *et al.* (1998)
MEFNEQ	Ru	NCMe	CO	−6.2 (2)	Ellis *et al.* (2000)
ZEPYIC	Ru[a]	Cl	CO	9.6 (3)	Anderson *et al.* (1995)

Notes: (*a*) in these compounds, the metallacarborane is monoanionic; (*b*) in this compound, the metallacarborane is monocationic; (*c*) the coordinates of *L* were taken as the mid-point of the C≡C bond.

Table 4
Selected geometric parameters (Å, °).

P1—Rh3	2.3789 (6)	C2—Rh3	2.208 (2)
N1—O32	1.231 (2)	Rh3—B4	2.219 (2)
N1—O33	1.234 (3)	Rh3—B7	2.256 (2)
C1—C2	1.639 (3)	Rh3—B8	2.243 (2)
C1—Rh3	2.184 (2)	Rh3—O31	2.1982 (14)
P2—Rh3	2.3931 (6)		
O32—N1—O31	117.74 (19)	O31—Rh3—P1	85.43 (4)
O32—N1—O33	122.3 (2)	O31—Rh3—P2	78.95 (5)
O33—N1—O31	119.99 (19)	N1—O31—Rh3	130.71 (14)
P1—Rh3—P2	99.23 (2)		

as before as $L—M—$cent1—cent2. It is clear that in all cases the θ values are close to zero (the fact that some are positive and some negative merely reflects the asymmetric unit deposited in the CSD). Thus, for all these molecules, as is the case with the title compound, there is a clearly preferred exopolyhedral ligand orientation in which the single weak exopolyhedral ligand lies *cis* to the cage C atoms.

The Rh1—O31 distance (Table 4) is 2.1982 (14) Å, close to the Rh—O distances of 2.209 (5) and 2.223 (5) Å in the κ^2-nitrato precursor (McAnaw *et al.*, 2013). In the present compound, the Rh—P distances are essentially equal [Rh1—P1 = 2.3789 (6) Å and Rh1—P2 = 2.3931 (6) Å], reflecting the symmetric ELO of the {P_2O} fragment. In the related compound 3-H-3,3-$(PPh_3)_2$-3,1,2-*closo*-$RhC_2B_9H_{11}$ (McAnaw *et al.*, 2013), the strongest exopolyhedral ligand is H, and the preferred ELO forces one of the PPh_3 ligands to lie essentially *cis* to the cage C atoms. In this latter compound, the Rh—P distances are consequently unequal, that to the P atom *cis* to C being 2.3568 (5) Å and that to the other P atom being significantly shorter at 2.2960 (5) Å.

There are four intramolecular hydrogen-bonding contacts involving the nitrate O atoms, *viz.* H2···O33 = 2.25 (3) Å, H112···O31 = 2.34 (3) Å, H212···O31 = 2.50 (3) Å and H212···O32 = 2.55 (3) Å. Whilst the first of these may contribute to the preference of the nitrate group to lie *cis* to the cage C atoms, we do not believe that it is the primary reason for this orientation (see discussion of ELO above). It may, however, be responsible for the 22.42 (8)° twist of the NO_3 ligand relative to the plane through atoms Rh3/B6/B8/B10.

The only significant intermolecular contacts are O32···H116*A* of 2.52 (3) Å [symmetry code: (*A*) $-x+1, -y+1, -z+1$] and H103···H9*B* of 2.22 (3) Å [symmetry code: (*B*) $-x+2, -y+2, -z+2$]. Whilst the former represents a weak hydrogen bond, the latter represents a weak dihydrogen bond since the BH units in carboranes and heterocarboranes are hydridic in nature.

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Computing details

Data collection: *APEX2* (Bruker, 2009); cell refinement: *APEX2* (Bruker, 2009); data reduction: *SAINT* (Bruker, 2009); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008) and *publCIF* (Westrip, 2010); program(s) used to refine structure: SHEXL2014 (Sheldrick, 2015); molecular graphics: OLEX2 (Dolomanov *et al.*, 2009); software used to prepare material for publication: OLEX2 (Dolomanov *et al.*, 2009).

3-(Nitrato-*κO*)-3,3-bis(triphenylphosphane-*κP*)-3-rhoda-\ 1,2-dicarba-*closo*-dodecaborane(11) dichloromethane 2.2-solvate

Crystal data

$[Rh(C_2H_{11}B_9)(NO_3)(C_{18}H_{15}P)_2]\cdot 2.2CH_2Cl_2$
M_r = 1008.69
Triclinic, $P\overline{1}$
a = 11.2934 (9) Å
b = 13.0083 (10) Å
c = 15.8655 (13) Å
α = 91.083 (4)°
β = 110.514 (4)°
γ = 99.713 (4)°
V = 2144.0 (3) Å^3
Z = 2
$F(000)$ = 1025
D_x = 1.562 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9956 reflections
θ = 2.4–28.3°
μ = 0.79 mm^{-1}
T = 100 K
PLATE, orange
0.56 × 0.32 × 0.08 mm

Data collection

Bruker APEXII CCD diffractometer
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
T_{min} = 0.660, T_{max} = 0.746
40881 measured reflections
10603 independent reflections
8793 reflections with $I > 2\sigma(I)$
R_{int} = 0.035
θ_{max} = 28.5°, θ_{min} = 2.2°
h = −15→14
k = −17→17
l = −21→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.089
S = 1.05
10597 reflections
520 parameters
0 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0442P)^2 + 1.0745P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$

$\Delta\rho_{max} = 1.04$ e Å^{-3}
$\Delta\rho_{min} = -0.74$ e Å^{-3}

Special details

Experimental. Absorption correction: SADABS-2008/1 (Bruker,2008) was used for absorption correction. wR2(int) was 0.0598 before and 0.0451 after correction. The ratio of minimum to maximum transmission is 0.8849.

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
P1	0.77241 (5)	0.67698 (4)	0.74878 (3)	0.01271 (11)
N1	0.87860 (18)	0.65330 (15)	0.52152 (13)	0.0215 (4)
C1	0.9582 (2)	0.92169 (16)	0.61657 (14)	0.0137 (4)
H1	0.997 (2)	0.8910 (19)	0.5816 (16)	0.016*
P2	1.10932 (5)	0.74601 (4)	0.77396 (4)	0.01356 (11)
C2	0.8018 (2)	0.88723 (17)	0.58661 (14)	0.0151 (4)
H2	0.765 (2)	0.841 (2)	0.5386 (17)	0.018*
Rh3	0.90764 (2)	0.79625 (2)	0.69438 (2)	0.01151 (5)
B4	1.0307 (2)	0.95430 (19)	0.73121 (17)	0.0167 (5)
H4	1.131 (2)	0.953 (2)	0.7639 (16)	0.020*
B5	1.0059 (3)	1.0516 (2)	0.64997 (17)	0.0194 (5)
H5	1.090 (2)	1.097 (2)	0.6397 (17)	0.023*
B6	0.8624 (3)	1.00666 (19)	0.55738 (17)	0.0184 (5)
H6	0.848 (2)	1.017 (2)	0.4851 (17)	0.022*
B7	0.7524 (2)	0.89183 (19)	0.67575 (16)	0.0149 (5)
H7	0.667 (2)	0.847 (2)	0.6730 (16)	0.018*
B8	0.8979 (2)	0.93764 (19)	0.77311 (16)	0.0161 (5)
H8	0.905 (2)	0.927 (2)	0.8480 (16)	0.019*
B9	0.9657 (3)	1.06382 (19)	0.74833 (17)	0.0186 (5)
H9	1.023 (2)	1.125 (2)	0.8029 (17)	0.022*
B10	0.8633 (3)	1.0969 (2)	0.64256 (17)	0.0195 (5)
H10	0.854 (2)	1.173 (2)	0.6309 (17)	0.023*
B11	0.7322 (3)	0.9899 (2)	0.59632 (17)	0.0188 (5)
H11	0.636 (2)	0.996 (2)	0.5488 (17)	0.023*
B12	0.7956 (3)	1.0254 (2)	0.71529 (17)	0.0186 (5)
H12	0.739 (2)	1.068 (2)	0.7481 (17)	0.022*
O31	0.89962 (15)	0.66171 (11)	0.60529 (11)	0.0190 (3)
O32	0.91609 (17)	0.58184 (14)	0.49219 (11)	0.0283 (4)
O33	0.8204 (2)	0.71454 (16)	0.47201 (12)	0.0383 (5)
C101	0.7601 (2)	0.73522 (16)	0.84977 (14)	0.0154 (4)
C102	0.8653 (2)	0.74040 (17)	0.93054 (14)	0.0164 (4)
H102	0.9351	0.7078	0.9320	0.020*
C103	0.8682 (2)	0.79282 (18)	1.00855 (15)	0.0208 (5)
H103	0.9397	0.7959	1.0632	0.025*

C104	0.7667 (2)	0.84065 (19)	1.00641 (16)	0.0238 (5)
H104	0.7685	0.8767	1.0596	0.029*
C105	0.6621 (2)	0.83591 (19)	0.92634 (16)	0.0234 (5)
H105	0.5929	0.8692	0.9251	0.028*
C106	0.6579 (2)	0.78303 (17)	0.84843 (15)	0.0179 (4)
H106	0.5856	0.7794	0.7942	0.022*
C107	0.7981 (2)	0.54445 (16)	0.77742 (14)	0.0148 (4)
C108	0.7805 (2)	0.50118 (18)	0.85334 (15)	0.0187 (4)
H108	0.7688	0.5446	0.8975	0.022*
C109	0.7799 (2)	0.39519 (18)	0.86463 (16)	0.0227 (5)
H109	0.7686	0.3666	0.9166	0.027*
C110	0.7958 (2)	0.33164 (18)	0.79988 (16)	0.0243 (5)
H110	0.7951	0.2593	0.8072	0.029*
C111	0.8127 (2)	0.37379 (18)	0.72415 (16)	0.0231 (5)
H111	0.8231	0.3299	0.6797	0.028*
C112	0.8146 (2)	0.47955 (17)	0.71287 (15)	0.0186 (4)
H112	0.8270	0.5078	0.6612	0.022*
C113	0.6081 (2)	0.63853 (17)	0.66624 (14)	0.0154 (4)
C114	0.5795 (2)	0.65316 (17)	0.57549 (15)	0.0185 (4)
H114	0.6447	0.6881	0.5556	0.022*
C115	0.4552 (2)	0.61682 (19)	0.51286 (16)	0.0233 (5)
H115	0.4363	0.6268	0.4507	0.028*
C116	0.3602 (2)	0.56643 (18)	0.54162 (16)	0.0229 (5)
H116	0.2754	0.5431	0.4994	0.028*
C117	0.3888 (2)	0.54987 (18)	0.63250 (16)	0.0218 (5)
H117	0.3237	0.5143	0.6521	0.026*
C118	0.5122 (2)	0.58524 (18)	0.69455 (16)	0.0201 (5)
H118	0.5315	0.5732	0.7564	0.024*
C201	1.1125 (2)	0.60599 (17)	0.78369 (14)	0.0155 (4)
C202	1.1095 (2)	0.56430 (18)	0.86388 (15)	0.0190 (5)
H202	1.1021	0.6079	0.9098	0.023*
C203	1.1172 (2)	0.45993 (19)	0.87707 (16)	0.0233 (5)
H203	1.1147	0.4324	0.9316	0.028*
C204	1.1285 (2)	0.39596 (19)	0.81007 (17)	0.0252 (5)
H204	1.1365	0.3252	0.8196	0.030*
C205	1.1282 (2)	0.43527 (18)	0.72979 (16)	0.0223 (5)
H205	1.1340	0.3909	0.6837	0.027*
C206	1.1193 (2)	0.53952 (18)	0.71585 (15)	0.0186 (4)
H206	1.1180	0.5656	0.6601	0.022*
C207	1.2198 (2)	0.79311 (17)	0.71462 (14)	0.0163 (4)
C208	1.3287 (2)	0.87055 (18)	0.75613 (16)	0.0214 (5)
H208	1.3480	0.8976	0.8164	0.026*
C209	1.4090 (2)	0.9083 (2)	0.71018 (17)	0.0258 (5)
H209	1.4825	0.9611	0.7393	0.031*
C210	1.3833 (2)	0.8699 (2)	0.62250 (17)	0.0258 (5)
H210	1.4395	0.8952	0.5917	0.031*
C211	1.2745 (2)	0.79390 (19)	0.57993 (16)	0.0215 (5)
H211	1.2558	0.7675	0.5195	0.026*

C212	1.1927 (2)	0.75624 (17)	0.62513 (14)	0.0170 (4)
H212	1.1177	0.7050	0.5950	0.020*
C213	1.2025 (2)	0.79606 (17)	0.89153 (14)	0.0173 (4)
C214	1.1578 (2)	0.85900 (17)	0.94137 (15)	0.0191 (5)
H214	1.0777	0.8805	0.9135	0.023*
C215	1.2303 (2)	0.89048 (18)	1.03202 (15)	0.0217 (5)
H215	1.1983	0.9322	1.0658	0.026*
C216	1.3480 (2)	0.86155 (19)	1.07301 (16)	0.0257 (5)
H216	1.3968	0.8833	1.1348	0.031*
C217	1.3952 (2)	0.80033 (19)	1.02359 (16)	0.0252 (5)
H217	1.4771	0.7816	1.0512	0.030*
C218	1.3221 (2)	0.76673 (19)	0.93362 (15)	0.0216 (5)
H218	1.3534	0.7236	0.9005	0.026*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
P1	0.0157 (3)	0.0113 (3)	0.0117 (2)	0.0039 (2)	0.0050 (2)	0.00183 (19)
N1	0.0206 (10)	0.0178 (10)	0.0248 (10)	0.0050 (8)	0.0059 (8)	0.0033 (8)
C1	0.0180 (10)	0.0117 (10)	0.0138 (10)	0.0050 (8)	0.0076 (8)	0.0046 (8)
P2	0.0155 (3)	0.0129 (3)	0.0126 (3)	0.0047 (2)	0.0044 (2)	0.0025 (2)
C2	0.0195 (11)	0.0135 (10)	0.0118 (10)	0.0059 (8)	0.0039 (8)	0.0025 (8)
Rh3	0.01449 (9)	0.00958 (8)	0.01125 (8)	0.00430 (6)	0.00461 (6)	0.00194 (6)
B4	0.0203 (12)	0.0104 (11)	0.0195 (12)	0.0028 (9)	0.0072 (10)	0.0027 (9)
B5	0.0282 (14)	0.0115 (12)	0.0200 (12)	0.0039 (10)	0.0103 (11)	0.0020 (9)
B6	0.0270 (13)	0.0138 (12)	0.0187 (12)	0.0083 (10)	0.0109 (11)	0.0079 (9)
B7	0.0196 (12)	0.0128 (11)	0.0141 (11)	0.0080 (9)	0.0060 (10)	0.0024 (9)
B8	0.0218 (12)	0.0135 (12)	0.0150 (11)	0.0082 (9)	0.0067 (10)	0.0024 (9)
B9	0.0279 (13)	0.0114 (11)	0.0177 (12)	0.0048 (10)	0.0090 (11)	0.0026 (9)
B10	0.0279 (14)	0.0133 (12)	0.0190 (12)	0.0075 (10)	0.0088 (11)	0.0025 (10)
B11	0.0250 (13)	0.0169 (12)	0.0160 (12)	0.0100 (10)	0.0063 (10)	0.0039 (9)
B12	0.0272 (13)	0.0163 (12)	0.0156 (12)	0.0097 (10)	0.0089 (10)	0.0035 (9)
O31	0.0262 (8)	0.0080 (7)	0.0302 (9)	0.0043 (6)	0.0186 (7)	−0.0006 (6)
O32	0.0341 (10)	0.0276 (10)	0.0256 (9)	0.0122 (8)	0.0111 (8)	−0.0055 (7)
O33	0.0647 (13)	0.0356 (11)	0.0199 (9)	0.0301 (10)	0.0120 (9)	0.0071 (8)
C101	0.0207 (11)	0.0120 (10)	0.0158 (10)	0.0035 (8)	0.0090 (9)	0.0031 (8)
C102	0.0182 (11)	0.0152 (10)	0.0171 (10)	0.0036 (8)	0.0076 (9)	0.0032 (8)
C103	0.0267 (12)	0.0187 (11)	0.0159 (11)	0.0028 (9)	0.0071 (9)	0.0020 (9)
C104	0.0349 (13)	0.0207 (12)	0.0199 (11)	0.0049 (10)	0.0149 (10)	−0.0001 (9)
C105	0.0282 (13)	0.0200 (12)	0.0268 (12)	0.0084 (10)	0.0140 (10)	0.0016 (10)
C106	0.0204 (11)	0.0161 (11)	0.0186 (11)	0.0056 (9)	0.0075 (9)	0.0045 (8)
C107	0.0146 (10)	0.0121 (10)	0.0164 (10)	0.0028 (8)	0.0037 (8)	0.0015 (8)
C108	0.0219 (11)	0.0166 (11)	0.0178 (11)	0.0045 (9)	0.0070 (9)	0.0032 (8)
C109	0.0273 (12)	0.0171 (11)	0.0227 (12)	0.0018 (9)	0.0084 (10)	0.0073 (9)
C110	0.0278 (12)	0.0119 (11)	0.0281 (12)	0.0026 (9)	0.0044 (10)	0.0036 (9)
C111	0.0289 (13)	0.0148 (11)	0.0235 (12)	0.0064 (9)	0.0061 (10)	−0.0020 (9)
C112	0.0236 (11)	0.0162 (11)	0.0150 (10)	0.0030 (9)	0.0060 (9)	0.0014 (8)
C113	0.0144 (10)	0.0133 (10)	0.0171 (10)	0.0048 (8)	0.0031 (8)	−0.0009 (8)

C114	0.0203 (11)	0.0156 (11)	0.0186 (11)	0.0023 (9)	0.0065 (9)	−0.0006 (8)
C115	0.0251 (12)	0.0240 (12)	0.0168 (11)	0.0037 (10)	0.0033 (9)	−0.0015 (9)
C116	0.0181 (11)	0.0178 (12)	0.0275 (12)	0.0053 (9)	0.0009 (10)	−0.0027 (9)
C117	0.0185 (11)	0.0177 (11)	0.0314 (13)	0.0032 (9)	0.0117 (10)	0.0024 (9)
C118	0.0218 (11)	0.0163 (11)	0.0217 (11)	0.0034 (9)	0.0073 (9)	0.0040 (9)
C201	0.0138 (10)	0.0143 (10)	0.0180 (10)	0.0058 (8)	0.0035 (8)	0.0037 (8)
C202	0.0220 (11)	0.0196 (11)	0.0176 (11)	0.0058 (9)	0.0086 (9)	0.0035 (9)
C203	0.0276 (12)	0.0223 (12)	0.0218 (12)	0.0089 (10)	0.0088 (10)	0.0107 (9)
C204	0.0315 (13)	0.0161 (11)	0.0308 (13)	0.0109 (10)	0.0111 (11)	0.0101 (10)
C205	0.0269 (12)	0.0188 (12)	0.0255 (12)	0.0073 (9)	0.0131 (10)	0.0025 (9)
C206	0.0207 (11)	0.0197 (11)	0.0184 (11)	0.0066 (9)	0.0091 (9)	0.0052 (9)
C207	0.0168 (10)	0.0173 (11)	0.0180 (10)	0.0083 (8)	0.0074 (9)	0.0087 (8)
C208	0.0215 (11)	0.0205 (12)	0.0209 (11)	0.0043 (9)	0.0057 (9)	0.0047 (9)
C209	0.0168 (11)	0.0267 (13)	0.0306 (13)	0.0032 (9)	0.0047 (10)	0.0097 (10)
C210	0.0222 (12)	0.0307 (14)	0.0327 (13)	0.0135 (10)	0.0149 (11)	0.0185 (11)
C211	0.0234 (12)	0.0268 (13)	0.0197 (11)	0.0131 (10)	0.0100 (9)	0.0103 (9)
C212	0.0168 (10)	0.0182 (11)	0.0189 (11)	0.0080 (8)	0.0077 (9)	0.0076 (8)
C213	0.0187 (11)	0.0158 (11)	0.0151 (10)	0.0024 (8)	0.0035 (9)	0.0033 (8)
C214	0.0227 (11)	0.0165 (11)	0.0169 (11)	0.0031 (9)	0.0058 (9)	0.0041 (8)
C215	0.0304 (13)	0.0166 (11)	0.0171 (11)	0.0023 (9)	0.0083 (10)	0.0009 (9)
C216	0.0308 (13)	0.0235 (13)	0.0156 (11)	−0.0022 (10)	0.0026 (10)	0.0024 (9)
C217	0.0221 (12)	0.0261 (13)	0.0218 (12)	0.0028 (10)	0.0015 (10)	0.0048 (10)
C218	0.0193 (11)	0.0273 (13)	0.0176 (11)	0.0069 (9)	0.0045 (9)	0.0038 (9)

Geometric parameters (Å, º)

P1—Rh3	2.3789 (6)	C104—C105	1.391 (4)
P1—C101	1.818 (2)	C105—H105	0.9500
P1—C107	1.836 (2)	C105—C106	1.385 (3)
P1—C113	1.835 (2)	C106—H106	0.9500
N1—O31	1.265 (2)	C107—C108	1.401 (3)
N1—O32	1.231 (2)	C107—C112	1.396 (3)
N1—O33	1.234 (3)	C108—H108	0.9500
C1—H1	0.93 (2)	C108—C109	1.393 (3)
C1—C2	1.639 (3)	C109—H109	0.9500
C1—Rh3	2.184 (2)	C109—C110	1.385 (3)
C1—B4	1.723 (3)	C110—H110	0.9500
C1—B5	1.698 (3)	C110—C111	1.390 (3)
C1—B6	1.734 (3)	C111—H111	0.9500
P2—Rh3	2.3931 (6)	C111—C112	1.388 (3)
P2—C201	1.836 (2)	C112—H112	0.9500
P2—C207	1.845 (2)	C113—C114	1.385 (3)
P2—C213	1.832 (2)	C113—C118	1.398 (3)
C2—H2	0.89 (3)	C114—H114	0.9500
C2—Rh3	2.208 (2)	C114—C115	1.401 (3)
C2—B6	1.729 (3)	C115—H115	0.9500
C2—B7	1.695 (3)	C115—C116	1.381 (3)
C2—B11	1.690 (3)	C116—H116	0.9500

Rh3—B4	2.219 (2)	C116—C117	1.392 (3)
Rh3—B7	2.256 (2)	C117—H117	0.9500
Rh3—B8	2.243 (2)	C117—C118	1.388 (3)
Rh3—O31	2.1982 (14)	C118—H118	0.9500
B4—H4	1.07 (3)	C201—C202	1.401 (3)
B4—B5	1.808 (4)	C201—C206	1.399 (3)
B4—B8	1.826 (4)	C202—H202	0.9500
B4—B9	1.767 (4)	C202—C203	1.390 (3)
B5—H5	1.10 (3)	C203—H203	0.9500
B5—B6	1.762 (4)	C203—C204	1.392 (3)
B5—B9	1.783 (4)	C204—H204	0.9500
B5—B10	1.773 (4)	C204—C205	1.380 (3)
B6—H6	1.11 (2)	C205—H205	0.9500
B6—B10	1.769 (4)	C205—C206	1.393 (3)
B6—B11	1.768 (4)	C206—H206	0.9500
B7—H7	1.02 (2)	C207—C208	1.397 (3)
B7—B8	1.816 (3)	C207—C212	1.400 (3)
B7—B11	1.796 (4)	C208—H208	0.9500
B7—B12	1.764 (3)	C208—C209	1.385 (3)
B8—H8	1.17 (2)	C209—H209	0.9500
B8—B9	1.802 (4)	C209—C210	1.382 (4)
B8—B12	1.795 (4)	C210—H210	0.9500
B9—H9	1.10 (2)	C210—C211	1.388 (4)
B9—B10	1.782 (4)	C211—H211	0.9500
B9—B12	1.782 (4)	C211—C212	1.390 (3)
B10—H10	1.02 (3)	C212—H212	0.9500
B10—B11	1.782 (4)	C213—C214	1.394 (3)
B10—B12	1.789 (4)	C213—C218	1.402 (3)
B11—H11	1.10 (3)	C214—H214	0.9500
B11—B12	1.788 (4)	C214—C215	1.395 (3)
B12—H12	1.15 (2)	C215—H215	0.9500
C101—C102	1.400 (3)	C215—C216	1.380 (4)
C101—C106	1.394 (3)	C216—H216	0.9500
C102—H102	0.9500	C216—C217	1.395 (4)
C102—C103	1.389 (3)	C217—H217	0.9500
C103—H103	0.9500	C217—C218	1.393 (3)
C103—C104	1.385 (3)	C218—H218	0.9500
C104—H104	0.9500		

C101—P1—Rh3	110.47 (7)	B10—B9—B12	60.26 (15)
C101—P1—C107	103.72 (10)	B12—B9—B5	107.79 (18)
C101—P1—C113	107.10 (10)	B12—B9—B8	60.12 (14)
C107—P1—Rh3	124.16 (7)	B12—B9—H9	123.2 (13)
C113—P1—Rh3	112.86 (7)	B5—B10—B9	60.20 (15)
C113—P1—C107	96.77 (10)	B5—B10—H10	121.8 (14)
O32—N1—O31	117.74 (19)	B5—B10—B11	107.49 (18)
O32—N1—O33	122.3 (2)	B5—B10—B12	107.91 (18)
O33—N1—O31	119.99 (19)	B6—B10—B5	59.66 (14)

C2—C1—H1	116.8 (15)	B6—B10—B9	107.85 (18)
C2—C1—Rh3	68.87 (11)	B6—B10—H10	122.0 (14)
C2—C1—B4	111.42 (16)	B6—B10—B11	59.72 (14)
C2—C1—B5	110.57 (17)	B6—B10—B12	107.82 (18)
C2—C1—B6	61.60 (14)	B9—B10—H10	121.6 (14)
Rh3—C1—H1	104.4 (15)	B9—B10—B11	107.87 (18)
B4—C1—H1	123.9 (15)	B9—B10—B12	59.88 (15)
B4—C1—Rh3	68.03 (11)	B11—B10—H10	122.0 (14)
B4—C1—B6	115.20 (17)	B11—B10—B12	60.10 (15)
B5—C1—H1	119.3 (15)	B12—B10—H10	121.8 (14)
B5—C1—Rh3	127.33 (14)	C2—B11—B6	59.93 (14)
B5—C1—B4	63.80 (14)	C2—B11—B7	58.11 (13)
B5—C1—B6	61.77 (14)	C2—B11—B10	104.58 (18)
B6—C1—H1	112.0 (15)	C2—B11—H11	121.2 (13)
B6—C1—Rh3	127.60 (14)	C2—B11—B12	102.95 (17)
C201—P2—Rh3	118.20 (7)	B6—B11—B7	108.97 (17)
C201—P2—C207	105.89 (10)	B6—B11—B10	59.79 (15)
C207—P2—Rh3	107.49 (7)	B6—B11—H11	118.7 (13)
C213—P2—Rh3	120.79 (7)	B6—B11—B12	107.91 (18)
C213—P2—C201	99.56 (10)	B7—B11—H11	120.9 (14)
C213—P2—C207	103.15 (10)	B10—B11—B7	107.76 (18)
C1—C2—H2	114.6 (16)	B10—B11—H11	125.2 (14)
C1—C2—Rh3	67.32 (10)	B10—B11—B12	60.15 (14)
C1—C2—B6	61.91 (14)	B12—B11—B7	58.96 (14)
C1—C2—B7	112.36 (16)	B12—B11—H11	126.9 (13)
C1—C2—B11	111.92 (17)	B7—B12—B8	61.34 (14)
Rh3—C2—H2	104.1 (17)	B7—B12—B9	108.44 (18)
B6—C2—H2	111.3 (16)	B7—B12—B10	108.87 (17)
B6—C2—Rh3	126.43 (14)	B7—B12—B11	60.74 (14)
B7—C2—H2	124.6 (16)	B7—B12—H12	124.4 (13)
B7—C2—Rh3	69.21 (11)	B8—B12—H12	123.0 (13)
B7—C2—B6	115.82 (17)	B9—B12—B8	60.49 (14)
B11—C2—H2	119.7 (17)	B9—B12—B10	59.86 (15)
B11—C2—Rh3	128.37 (14)	B9—B12—B11	107.58 (17)
B11—C2—B6	62.28 (15)	B9—B12—H12	120.6 (13)
B11—C2—B7	64.07 (14)	B10—B12—B8	109.85 (18)
P1—Rh3—P2	99.23 (2)	B10—B12—H12	117.2 (13)
C1—Rh3—P1	157.40 (6)	B11—B12—B8	110.37 (17)
C1—Rh3—P2	103.37 (6)	B11—B12—B10	59.75 (14)
C1—Rh3—C2	43.81 (8)	B11—B12—H12	120.1 (13)
C1—Rh3—B4	46.07 (9)	N1—O31—Rh3	130.71 (14)
C1—Rh3—B7	77.18 (9)	C102—C101—P1	117.22 (16)
C1—Rh3—B8	78.75 (8)	C106—C101—P1	123.19 (17)
C1—Rh3—O31	98.65 (7)	C106—C101—C102	119.29 (19)
C2—Rh3—P1	113.77 (6)	C101—C102—H102	119.8
C2—Rh3—P2	146.33 (6)	C103—C102—C101	120.5 (2)
C2—Rh3—B4	77.74 (9)	C103—C102—H102	119.8
C2—Rh3—B7	44.62 (8)	C102—C103—H103	120.1

C2—Rh3—B8	77.71 (8)	C104—C103—C102	119.8 (2)
B4—Rh3—P1	139.94 (7)	C104—C103—H103	120.1
B4—Rh3—P2	81.33 (7)	C103—C104—H104	120.0
B4—Rh3—B7	81.22 (9)	C103—C104—C105	120.0 (2)
B4—Rh3—B8	48.30 (9)	C105—C104—H104	120.0
B7—Rh3—P1	82.54 (7)	C104—C105—H105	119.7
B7—Rh3—P2	154.43 (6)	C106—C105—C104	120.6 (2)
B8—Rh3—P1	94.89 (7)	C106—C105—H105	119.7
B8—Rh3—P2	107.01 (7)	C101—C106—H106	120.1
B8—Rh3—B7	47.59 (9)	C105—C106—C101	119.9 (2)
O31—Rh3—P1	85.43 (4)	C105—C106—H106	120.1
O31—Rh3—P2	78.95 (5)	C108—C107—P1	122.52 (16)
O31—Rh3—C2	96.54 (7)	C112—C107—P1	117.62 (16)
O31—Rh3—B4	133.01 (8)	C112—C107—C108	119.0 (2)
O31—Rh3—B7	126.52 (8)	C107—C108—H108	119.7
O31—Rh3—B8	173.86 (8)	C109—C108—C107	120.6 (2)
C1—B4—Rh3	65.90 (11)	C109—C108—H108	119.7
C1—B4—H4	119.7 (13)	C108—C109—H109	120.1
C1—B4—B5	57.44 (13)	C110—C109—C108	119.8 (2)
C1—B4—B8	104.62 (17)	C110—C109—H109	120.1
C1—B4—B9	103.14 (17)	C109—C110—H110	120.0
Rh3—B4—H4	113.8 (14)	C109—C110—C111	120.0 (2)
B5—B4—Rh3	119.58 (15)	C111—C110—H110	120.0
B5—B4—H4	111.1 (14)	C110—C111—H111	119.7
B5—B4—B8	108.24 (17)	C112—C111—C110	120.6 (2)
B8—B4—Rh3	66.55 (11)	C112—C111—H111	119.7
B8—B4—H4	131.7 (13)	C107—C112—H112	120.0
B9—B4—Rh3	120.33 (16)	C111—C112—C107	120.1 (2)
B9—B4—H4	120.9 (13)	C111—C112—H112	120.0
B9—B4—B5	59.81 (14)	C114—C113—P1	121.47 (17)
B9—B4—B8	60.18 (14)	C114—C113—C118	119.3 (2)
C1—B5—B4	58.76 (13)	C118—C113—P1	118.97 (17)
C1—B5—H5	121.1 (13)	C113—C114—H114	119.8
C1—B5—B6	60.09 (14)	C113—C114—C115	120.4 (2)
C1—B5—B9	103.47 (18)	C115—C114—H114	119.8
C1—B5—B10	105.25 (18)	C114—C115—H115	120.0
B4—B5—H5	118.8 (14)	C116—C115—C114	119.9 (2)
B6—B5—B4	109.65 (18)	C116—C115—H115	120.0
B6—B5—H5	120.4 (13)	C115—C116—H116	120.0
B6—B5—B9	108.13 (19)	C115—C116—C117	120.0 (2)
B6—B5—B10	60.07 (15)	C117—C116—H116	120.0
B9—B5—B4	58.93 (14)	C116—C117—H117	119.9
B9—B5—H5	125.4 (13)	C118—C117—C116	120.2 (2)
B10—B5—B4	108.17 (18)	C118—C117—H117	119.9
B10—B5—H5	125.8 (14)	C113—C118—H118	119.9
B10—B5—B9	60.14 (15)	C117—C118—C113	120.2 (2)
C1—B6—B5	58.13 (14)	C117—C118—H118	119.9
C1—B6—H6	120.8 (13)	C202—C201—P2	117.99 (16)

C1—B6—B10	103.93 (17)	C206—C201—P2	123.43 (17)
C1—B6—B11	103.95 (17)	C206—C201—C202	118.6 (2)
C2—B6—C1	56.50 (13)	C201—C202—H202	119.6
C2—B6—B5	103.61 (17)	C203—C202—C201	120.8 (2)
C2—B6—H6	119.0 (13)	C203—C202—H202	119.6
C2—B6—B10	103.50 (17)	C202—C203—H203	120.1
C2—B6—B11	57.79 (14)	C202—C203—C204	119.7 (2)
B5—B6—H6	125.8 (13)	C204—C203—H203	120.1
B5—B6—B10	60.28 (15)	C203—C204—H204	120.0
B5—B6—B11	108.59 (18)	C205—C204—C203	120.1 (2)
B10—B6—H6	129.9 (13)	C205—C204—H204	120.0
B11—B6—H6	121.7 (13)	C204—C205—H205	119.8
B11—B6—B10	60.49 (15)	C204—C205—C206	120.5 (2)
C2—B7—Rh3	66.17 (11)	C206—C205—H205	119.8
C2—B7—H7	120.6 (13)	C201—C206—H206	119.9
C2—B7—B8	105.33 (17)	C205—C206—C201	120.3 (2)
C2—B7—B11	57.82 (13)	C205—C206—H206	119.9
C2—B7—B12	103.76 (17)	C208—C207—P2	120.85 (17)
Rh3—B7—H7	112.7 (14)	C208—C207—C212	118.3 (2)
B8—B7—Rh3	65.82 (11)	C212—C207—P2	120.77 (17)
B8—B7—H7	129.2 (14)	C207—C208—H208	119.7
B11—B7—Rh3	119.97 (15)	C209—C208—C207	120.6 (2)
B11—B7—H7	113.0 (14)	C209—C208—H208	119.7
B11—B7—B8	109.10 (18)	C208—C209—H209	119.6
B12—B7—Rh3	119.56 (15)	C210—C209—C208	120.8 (2)
B12—B7—H7	121.5 (14)	C210—C209—H209	119.6
B12—B7—B8	60.19 (14)	C209—C210—H210	120.4
B12—B7—B11	60.30 (14)	C209—C210—C211	119.3 (2)
Rh3—B8—H8	116.4 (12)	C211—C210—H210	120.4
B4—B8—Rh3	65.14 (10)	C210—C211—H211	119.8
B4—B8—H8	126.6 (12)	C210—C211—C212	120.4 (2)
B7—B8—Rh3	66.58 (10)	C212—C211—H211	119.8
B7—B8—B4	106.26 (16)	C207—C212—H212	119.7
B7—B8—H8	123.6 (12)	C211—C212—C207	120.6 (2)
B9—B8—Rh3	117.42 (14)	C211—C212—H212	119.7
B9—B8—B4	58.28 (14)	C214—C213—P2	122.89 (17)
B9—B8—B7	105.34 (17)	C214—C213—C218	118.9 (2)
B9—B8—H8	117.6 (12)	C218—C213—P2	118.18 (16)
B12—B8—Rh3	118.74 (14)	C213—C214—H214	119.9
B12—B8—B4	105.78 (17)	C213—C214—C215	120.3 (2)
B12—B8—B7	58.47 (14)	C215—C214—H214	119.9
B12—B8—H8	115.3 (12)	C214—C215—H215	119.7
B12—B8—B9	59.39 (14)	C216—C215—C214	120.5 (2)
B4—B9—B5	61.26 (14)	C216—C215—H215	119.7
B4—B9—B8	61.54 (14)	C215—C216—H216	120.1
B4—B9—H9	119.7 (14)	C215—C216—C217	119.9 (2)
B4—B9—B10	109.66 (17)	C217—C216—H216	120.1
B4—B9—B12	108.93 (18)	C216—C217—H217	120.1

B5—B9—B8	110.46 (17)	C218—C217—C216	119.8 (2)
B5—B9—H9	120.0 (13)	C218—C217—H217	120.1
B8—B9—H9	120.8 (14)	C213—C218—H218	119.7
B10—B9—B5	59.66 (15)	C217—C218—C213	120.5 (2)
B10—B9—B8	109.89 (18)	C217—C218—H218	119.7
B10—B9—H9	120.9 (14)		

P1—C101—C102—C103	173.70 (17)	B5—B9—B12—B8	103.83 (18)
P1—C101—C106—C105	−172.80 (18)	B5—B9—B12—B10	−37.42 (17)
P1—C107—C108—C109	169.21 (18)	B5—B9—B12—B11	−0.1 (2)
P1—C107—C112—C111	−169.17 (17)	B5—B10—B11—C2	4.2 (2)
P1—C113—C114—C115	175.69 (18)	B5—B10—B11—B6	−37.13 (17)
P1—C113—C118—C117	−176.25 (17)	B5—B10—B11—B7	64.9 (2)
C1—C2—B6—B5	−35.74 (15)	B5—B10—B11—B12	100.99 (19)
C1—C2—B6—B10	−97.93 (18)	B5—B10—B12—B7	−63.2 (2)
C1—C2—B6—B11	−139.34 (17)	B5—B10—B12—B8	2.3 (2)
C1—C2—B7—Rh3	−52.97 (14)	B5—B10—B12—B9	37.69 (17)
C1—C2—B7—B8	1.2 (2)	B5—B10—B12—B11	−100.28 (19)
C1—C2—B7—B11	104.41 (19)	B6—C1—C2—Rh3	−162.30 (13)
C1—C2—B7—B12	63.6 (2)	B6—C1—C2—B7	−108.31 (19)
C1—C2—B11—B6	38.29 (17)	B6—C1—C2—B11	−38.44 (17)
C1—C2—B11—B7	−105.09 (18)	B6—C1—B4—Rh3	122.50 (16)
C1—C2—B11—B10	−3.0 (2)	B6—C1—B4—B5	−35.51 (18)
C1—C2—B11—B12	−65.1 (2)	B6—C1—B4—B8	67.0 (2)
C1—B4—B5—B6	33.30 (16)	B6—C1—B4—B9	4.9 (2)
C1—B4—B5—B9	133.12 (19)	B6—C1—B5—B4	143.38 (18)
C1—B4—B5—B10	97.17 (19)	B6—C1—B5—B9	103.37 (19)
C1—B4—B8—Rh3	55.04 (12)	B6—C1—B5—B10	41.11 (16)
C1—B4—B8—B7	1.3 (2)	B6—C2—B7—Rh3	−121.46 (17)
C1—B4—B8—B9	−96.97 (18)	B6—C2—B7—B8	−67.3 (2)
C1—B4—B8—B12	−59.78 (19)	B6—C2—B7—B11	35.92 (18)
C1—B4—B9—B5	−39.18 (16)	B6—C2—B7—B12	−4.9 (2)
C1—B4—B9—B8	99.49 (17)	B6—C2—B11—B7	−143.38 (18)
C1—B4—B9—B10	−3.1 (2)	B6—C2—B11—B10	−41.29 (16)
C1—B4—B9—B12	61.2 (2)	B6—C2—B11—B12	−103.39 (19)
C1—B5—B6—C2	34.99 (15)	B6—B5—B9—B4	102.47 (19)
C1—B5—B6—B10	132.95 (18)	B6—B5—B9—B8	64.2 (2)
C1—B5—B6—B11	95.18 (18)	B6—B5—B9—B10	−37.50 (17)
C1—B5—B9—B4	39.92 (16)	B6—B5—B9—B12	0.2 (2)
C1—B5—B9—B8	1.6 (2)	B6—B5—B10—B9	138.12 (19)
C1—B5—B9—B10	−100.05 (19)	B6—B5—B10—B11	37.15 (17)
C1—B5—B9—B12	−62.4 (2)	B6—B5—B10—B12	100.58 (19)
C1—B5—B10—B6	−41.12 (16)	B6—B10—B11—C2	41.36 (16)
C1—B5—B10—B9	97.00 (19)	B6—B10—B11—B7	102.03 (18)
C1—B5—B10—B11	−4.0 (2)	B6—B10—B11—B12	138.12 (18)
C1—B5—B10—B12	59.5 (2)	B6—B10—B12—B7	−0.1 (2)
C1—B6—B10—B5	39.83 (16)	B6—B10—B12—B8	65.3 (2)
C1—B6—B10—B9	2.3 (2)	B6—B10—B12—B9	100.70 (19)

C1—B6—B10—B11	−98.33 (18)	B6—B10—B12—B11	−37.27 (17)
C1—B6—B10—B12	−60.9 (2)	B6—B11—B12—B7	−101.78 (19)
C1—B6—B11—C2	−34.04 (15)	B6—B11—B12—B8	−64.4 (2)
C1—B6—B11—B7	−1.7 (2)	B6—B11—B12—B9	−0.1 (2)
C1—B6—B11—B10	98.31 (18)	B6—B11—B12—B10	37.32 (17)
C1—B6—B11—B12	60.8 (2)	B7—C2—B6—C1	102.76 (19)
P2—C201—C202—C203	−177.24 (18)	B7—C2—B6—B5	67.0 (2)
P2—C201—C206—C205	176.63 (17)	B7—C2—B6—B10	4.8 (2)
P2—C207—C208—C209	−177.74 (18)	B7—C2—B6—B11	−36.58 (18)
P2—C207—C212—C211	178.36 (17)	B7—C2—B11—B6	143.38 (18)
P2—C213—C214—C215	176.81 (18)	B7—C2—B11—B10	102.08 (18)
P2—C213—C218—C217	−178.32 (19)	B7—C2—B11—B12	39.99 (16)
C2—C1—B4—Rh3	54.84 (14)	B7—B8—B9—B4	−99.89 (17)
C2—C1—B4—B5	−103.16 (19)	B7—B8—B9—B5	−61.7 (2)
C2—C1—B4—B8	−0.6 (2)	B7—B8—B9—B10	2.3 (2)
C2—C1—B4—B9	−62.8 (2)	B7—B8—B9—B12	37.60 (15)
C2—C1—B5—B4	104.48 (18)	B7—B8—B12—B9	−136.35 (18)
C2—C1—B5—B6	−38.90 (17)	B7—B8—B12—B10	−101.22 (19)
C2—C1—B5—B9	64.5 (2)	B7—B8—B12—B11	−37.14 (17)
C2—C1—B5—B10	2.2 (2)	B7—B11—B12—B8	37.40 (17)
C2—C1—B6—B5	138.05 (18)	B7—B11—B12—B9	101.70 (19)
C2—C1—B6—B10	97.14 (18)	B7—B11—B12—B10	139.10 (19)
C2—C1—B6—B11	34.62 (15)	B8—B4—B5—C1	−96.01 (18)
C2—B6—B10—B5	98.14 (18)	B8—B4—B5—B6	−62.7 (2)
C2—B6—B10—B9	60.7 (2)	B8—B4—B5—B9	37.11 (16)
C2—B6—B10—B11	−40.02 (16)	B8—B4—B5—B10	1.2 (2)
C2—B6—B10—B12	−2.6 (2)	B8—B4—B9—B5	−138.67 (18)
C2—B6—B11—B7	32.38 (16)	B8—B4—B9—B10	−102.5 (2)
C2—B6—B11—B10	132.35 (18)	B8—B4—B9—B12	−38.28 (16)
C2—B6—B11—B12	94.87 (19)	B8—B7—B11—C2	96.47 (18)
C2—B7—B8—Rh3	−54.39 (13)	B8—B7—B11—B6	63.4 (2)
C2—B7—B8—B4	−1.5 (2)	B8—B7—B11—B10	0.0 (2)
C2—B7—B8—B9	59.3 (2)	B8—B7—B11—B12	−36.57 (16)
C2—B7—B8—B12	97.31 (18)	B8—B7—B12—B9	39.29 (17)
C2—B7—B11—B6	−33.09 (16)	B8—B7—B12—B10	102.84 (19)
C2—B7—B11—B10	−96.43 (19)	B8—B7—B12—B11	139.54 (18)
C2—B7—B11—B12	−133.03 (19)	B8—B9—B10—B5	−102.66 (19)
C2—B7—B12—B8	−99.98 (17)	B8—B9—B10—B6	−65.4 (2)
C2—B7—B12—B9	−60.7 (2)	B8—B9—B10—B11	−2.3 (2)
C2—B7—B12—B10	2.9 (2)	B8—B9—B10—B12	35.25 (16)
C2—B7—B12—B11	39.57 (16)	B8—B9—B12—B7	−39.68 (16)
C2—B11—B12—B7	−39.55 (16)	B8—B9—B12—B10	−141.25 (17)
C2—B11—B12—B8	−2.2 (2)	B8—B9—B12—B11	−103.90 (18)
C2—B11—B12—B9	62.1 (2)	B9—B4—B5—C1	−133.12 (19)
C2—B11—B12—B10	99.55 (19)	B9—B4—B5—B6	−99.8 (2)
Rh3—P1—C101—C102	−76.38 (17)	B9—B4—B5—B10	−35.95 (17)
Rh3—P1—C101—C106	97.27 (18)	B9—B4—B8—Rh3	152.01 (15)
Rh3—P1—C107—C108	139.30 (16)	B9—B4—B8—B7	98.26 (18)

Rh3—P1—C107—C112	−51.64 (19)	B9—B4—B8—B12	37.19 (16)
Rh3—P1—C113—C114	17.7 (2)	B9—B5—B6—C1	−95.42 (19)
Rh3—P1—C113—C118	−167.90 (15)	B9—B5—B6—C2	−60.4 (2)
Rh3—C1—C2—B6	162.30 (13)	B9—B5—B6—B10	37.53 (17)
Rh3—C1—C2—B7	53.99 (14)	B9—B5—B6—B11	−0.2 (2)
Rh3—C1—C2—B11	123.85 (16)	B9—B5—B10—B6	−138.12 (19)
Rh3—C1—B4—B5	−158.01 (15)	B9—B5—B10—B11	−100.96 (19)
Rh3—C1—B4—B8	−55.45 (12)	B9—B5—B10—B12	−37.54 (17)
Rh3—C1—B4—B9	−117.62 (15)	B9—B8—B12—B7	136.35 (18)
Rh3—C1—B5—B4	25.90 (17)	B9—B8—B12—B10	35.13 (17)
Rh3—C1—B5—B6	−117.49 (19)	B9—B8—B12—B11	99.2 (2)
Rh3—C1—B5—B9	−14.1 (2)	B9—B10—B11—C2	−59.3 (2)
Rh3—C1—B5—B10	−76.4 (2)	B9—B10—B11—B6	−100.64 (19)
Rh3—C1—B6—C2	−20.98 (16)	B9—B10—B11—B7	1.4 (2)
Rh3—C1—B6—B5	117.08 (19)	B9—B10—B11—B12	37.48 (16)
Rh3—C1—B6—B10	76.2 (2)	B9—B10—B12—B7	−100.84 (19)
Rh3—C1—B6—B11	13.6 (2)	B9—B10—B12—B8	−35.39 (16)
Rh3—P2—C201—C202	−98.22 (17)	B9—B10—B12—B11	−137.97 (18)
Rh3—P2—C201—C206	82.64 (19)	B10—B5—B6—C1	−132.95 (18)
Rh3—P2—C207—C208	114.23 (18)	B10—B5—B6—C2	−97.96 (18)
Rh3—P2—C207—C212	−62.25 (18)	B10—B5—B6—B11	−37.77 (17)
Rh3—P2—C213—C214	4.2 (2)	B10—B5—B9—B4	139.97 (19)
Rh3—P2—C213—C218	−177.81 (15)	B10—B5—B9—B8	101.7 (2)
Rh3—C2—B6—C1	20.41 (15)	B10—B5—B9—B12	37.69 (17)
Rh3—C2—B6—B5	−15.3 (2)	B10—B6—B11—C2	−132.35 (18)
Rh3—C2—B6—B10	−77.5 (2)	B10—B6—B11—B7	−99.97 (19)
Rh3—C2—B6—B11	−118.93 (18)	B10—B6—B11—B12	−37.48 (17)
Rh3—C2—B7—B8	54.18 (13)	B10—B9—B12—B7	101.57 (18)
Rh3—C2—B7—B11	157.38 (15)	B10—B9—B12—B8	141.25 (17)
Rh3—C2—B7—B12	116.55 (15)	B10—B9—B12—B11	37.35 (17)
Rh3—C2—B11—B6	116.1 (2)	B10—B11—B12—B7	−139.10 (18)
Rh3—C2—B11—B7	−27.30 (18)	B10—B11—B12—B8	−101.7 (2)
Rh3—C2—B11—B10	74.8 (2)	B10—B11—B12—B9	−37.40 (17)
Rh3—C2—B11—B12	12.7 (3)	B11—C2—B6—C1	139.34 (17)
Rh3—B4—B5—C1	−23.15 (15)	B11—C2—B6—B5	103.60 (18)
Rh3—B4—B5—B6	10.2 (2)	B11—C2—B6—B10	41.41 (16)
Rh3—B4—B5—B9	109.97 (18)	B11—C2—B7—Rh3	−157.38 (15)
Rh3—B4—B5—B10	74.0 (2)	B11—C2—B7—B8	−103.20 (18)
Rh3—B4—B8—B7	−53.75 (13)	B11—C2—B7—B12	−40.82 (17)
Rh3—B4—B8—B9	−152.01 (15)	B11—B6—B10—B5	138.16 (19)
Rh3—B4—B8—B12	−114.82 (15)	B11—B6—B10—B9	100.7 (2)
Rh3—B4—B9—B5	−108.74 (19)	B11—B6—B10—B12	37.44 (17)
Rh3—B4—B9—B8	29.92 (16)	B11—B7—B8—Rh3	−115.09 (15)
Rh3—B4—B9—B10	−72.6 (2)	B11—B7—B8—B4	−62.2 (2)
Rh3—B4—B9—B12	−8.4 (2)	B11—B7—B8—B9	−1.4 (2)
Rh3—B7—B8—B4	52.88 (13)	B11—B7—B8—B12	36.62 (16)
Rh3—B7—B8—B9	113.68 (15)	B11—B7—B12—B8	−139.54 (18)
Rh3—B7—B8—B12	151.71 (15)	B11—B7—B12—B9	−100.26 (19)

Rh3—B7—B11—C2	23.97 (15)	B11—B7—B12—B10	−36.71 (17)
Rh3—B7—B11—B6	−9.1 (2)	B11—B10—B12—B7	37.13 (17)
Rh3—B7—B11—B10	−72.5 (2)	B11—B10—B12—B8	102.58 (19)
Rh3—B7—B11—B12	−109.07 (18)	B11—B10—B12—B9	137.97 (18)
Rh3—B7—B12—B8	−29.81 (15)	B12—B7—B8—Rh3	−151.71 (15)
Rh3—B7—B12—B9	9.5 (2)	B12—B7—B8—B4	−98.82 (18)
Rh3—B7—B12—B10	73.0 (2)	B12—B7—B8—B9	−38.03 (16)
Rh3—B7—B12—B11	109.73 (18)	B12—B7—B11—C2	133.03 (19)
Rh3—B8—B9—B4	−28.67 (15)	B12—B7—B11—B6	99.9 (2)
Rh3—B8—B9—B5	9.5 (2)	B12—B7—B11—B10	36.60 (17)
Rh3—B8—B9—B10	73.5 (2)	B12—B8—B9—B4	−137.48 (17)
Rh3—B8—B9—B12	108.82 (17)	B12—B8—B9—B5	−99.3 (2)
Rh3—B8—B12—B7	29.74 (16)	B12—B8—B9—B10	−35.30 (16)
Rh3—B8—B12—B9	−106.61 (17)	B12—B9—B10—B5	−137.90 (18)
Rh3—B8—B12—B10	−71.5 (2)	B12—B9—B10—B6	−100.66 (19)
Rh3—B8—B12—B11	−7.4 (2)	B12—B9—B10—B11	−37.58 (16)
B4—C1—C2—Rh3	−54.37 (14)	B12—B10—B11—C2	−96.76 (18)
B4—C1—C2—B6	107.92 (18)	B12—B10—B11—B6	−138.12 (18)
B4—C1—C2—B7	−0.4 (2)	B12—B10—B11—B7	−36.09 (16)
B4—C1—C2—B11	69.5 (2)	O32—N1—O31—Rh3	158.66 (15)
B4—C1—B5—B6	−143.38 (18)	O33—N1—O31—Rh3	−22.5 (3)
B4—C1—B5—B9	−40.01 (17)	C101—P1—C107—C108	12.4 (2)
B4—C1—B5—B10	−102.28 (19)	C101—P1—C107—C112	−178.56 (17)
B4—C1—B6—C2	−101.79 (19)	C101—P1—C113—C114	139.44 (18)
B4—C1—B6—B5	36.26 (18)	C101—P1—C113—C118	−46.1 (2)
B4—C1—B6—B10	−4.7 (2)	C101—C102—C103—C104	−0.2 (3)
B4—C1—B6—B11	−67.2 (2)	C102—C101—C106—C105	0.7 (3)
B4—B5—B6—C1	−32.79 (16)	C102—C103—C104—C105	0.1 (4)
B4—B5—B6—C2	2.2 (2)	C103—C104—C105—C106	0.4 (4)
B4—B5—B6—B10	100.2 (2)	C104—C105—C106—C101	−0.8 (4)
B4—B5—B6—B11	62.4 (2)	C106—C101—C102—C103	−0.2 (3)
B4—B5—B9—B8	−38.30 (17)	C107—P1—C101—C102	58.69 (19)
B4—B5—B9—B10	−139.97 (19)	C107—P1—C101—C106	−127.66 (19)
B4—B5—B9—B12	−102.28 (19)	C107—P1—C113—C114	−113.92 (19)
B4—B5—B10—B6	−102.68 (19)	C107—P1—C113—C118	60.53 (19)
B4—B5—B10—B9	35.44 (17)	C107—C108—C109—C110	−0.5 (3)
B4—B5—B10—B11	−65.5 (2)	C108—C107—C112—C111	0.3 (3)
B4—B5—B10—B12	−2.1 (2)	C108—C109—C110—C111	0.2 (4)
B4—B8—B9—B5	38.17 (17)	C109—C110—C111—C112	0.4 (4)
B4—B8—B9—B10	102.18 (19)	C110—C111—C112—C107	−0.6 (3)
B4—B8—B9—B12	137.48 (17)	C112—C107—C108—C109	0.3 (3)
B4—B8—B12—B7	99.67 (17)	C113—P1—C101—C102	160.35 (17)
B4—B8—B12—B9	−36.68 (15)	C113—P1—C101—C106	−26.0 (2)
B4—B8—B12—B10	−1.5 (2)	C113—P1—C107—C108	−97.11 (19)
B4—B8—B12—B11	62.5 (2)	C113—P1—C107—C112	71.94 (18)
B4—B9—B10—B5	−36.79 (17)	C113—C114—C115—C116	0.2 (3)
B4—B9—B10—B6	0.5 (2)	C114—C113—C118—C117	−1.7 (3)
B4—B9—B10—B11	63.5 (2)	C114—C115—C116—C117	−1.3 (4)

B4—B9—B10—B12	101.11 (19)	C115—C116—C117—C118	0.9 (3)
B4—B9—B12—B7	−0.8 (2)	C116—C117—C118—C113	0.6 (3)
B4—B9—B12—B8	38.91 (16)	C118—C113—C114—C115	1.3 (3)
B4—B9—B12—B10	−102.34 (19)	C201—P2—C207—C208	−118.55 (19)
B4—B9—B12—B11	−65.0 (2)	C201—P2—C207—C212	64.97 (19)
B5—C1—C2—Rh3	−123.32 (15)	C201—P2—C213—C214	−126.9 (2)
B5—C1—C2—B6	38.98 (17)	C201—P2—C213—C218	51.0 (2)
B5—C1—C2—B7	−69.3 (2)	C201—C202—C203—C204	0.3 (4)
B5—C1—C2—B11	0.5 (2)	C202—C201—C206—C205	−2.5 (3)
B5—C1—B4—Rh3	158.01 (15)	C202—C203—C204—C205	−2.0 (4)
B5—C1—B4—B8	102.55 (18)	C203—C204—C205—C206	1.4 (4)
B5—C1—B4—B9	40.38 (17)	C204—C205—C206—C201	0.9 (4)
B5—C1—B6—C2	−138.05 (18)	C206—C201—C202—C203	1.9 (3)
B5—C1—B6—B10	−40.91 (17)	C207—P2—C201—C202	141.30 (17)
B5—C1—B6—B11	−103.44 (19)	C207—P2—C201—C206	−37.8 (2)
B5—B4—B8—Rh3	115.06 (16)	C207—P2—C213—C214	124.14 (19)
B5—B4—B8—B7	61.3 (2)	C207—P2—C213—C218	−57.9 (2)
B5—B4—B8—B9	−36.95 (16)	C207—C208—C209—C210	−0.3 (4)
B5—B4—B8—B12	0.2 (2)	C208—C207—C212—C211	1.8 (3)
B5—B4—B9—B8	138.67 (18)	C208—C209—C210—C211	1.1 (4)
B5—B4—B9—B10	36.13 (18)	C209—C210—C211—C212	−0.5 (4)
B5—B4—B9—B12	100.39 (19)	C210—C211—C212—C207	−1.0 (3)
B5—B6—B10—B9	−37.49 (18)	C212—C207—C208—C209	−1.2 (3)
B5—B6—B10—B11	−138.16 (19)	C213—P2—C201—C202	34.57 (19)
B5—B6—B10—B12	−100.7 (2)	C213—P2—C201—C206	−144.57 (19)
B5—B6—B11—C2	−94.68 (19)	C213—P2—C207—C208	−14.4 (2)
B5—B6—B11—B7	−62.3 (2)	C213—P2—C207—C212	169.08 (18)
B5—B6—B11—B10	37.67 (17)	C213—C214—C215—C216	1.3 (3)
B5—B6—B11—B12	0.2 (2)	C214—C213—C218—C217	−0.3 (3)
B5—B9—B10—B6	37.25 (17)	C214—C215—C216—C217	0.0 (4)
B5—B9—B10—B11	100.33 (19)	C215—C216—C217—C218	−1.4 (4)
B5—B9—B10—B12	137.90 (18)	C216—C217—C218—C213	1.6 (4)
B5—B9—B12—B7	64.2 (2)	C218—C213—C214—C215	−1.1 (3)

Selected geometric parameters (Å, °).

Rh3—C1	2.184 (2)	Rh3—P1	2.3789 (6)
Rh3—C2	2.208 (2)	Rh3—P2	2.3931 (6)
Rh3—B7	2.256 (2)	Rh3—O31	2.1982 (14)
Rh3—B8	2.243 (2)	O31—N1	1.265 (2)
Rh3—B4	2.219 (2)	N1—O32	1.231 (2)
C1—C2	1.639 (3)	N1—O33	1.234 (3)
P1—Rh3—P2	99.23 (2)	O31—N1—O32	117.74 (19)
P1—Rh3—O31	85.43 (4)	O31—N1—O33	119.99 (19)
P2—Rh3—O31	78.95 (5)	O32—N1—O33	122.3 (2)
Rh3—O31—N1	130.71 (14)		